



Sample name: **M13_octanol** Experiment start time: **3/16/2018 8:34:17 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-16016** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

pH-metric Result

logP (XH +) -7.57 ±1.49 (n=50)
logP (neutral X) 2.89 ±0.02 (n=50)
RMSD 3.854

18C-16016 Points 2 to 15

M13_octanol concentration factor 0.878
Carbonate 0.0003 mM
Acidity error 2.29946 mM

18C-16016 Points 16 to 39

M13_octanol concentration factor 0.780
Carbonate 0.0000 mM
Acidity error 2.26129 mM

18C-16016 Points 40 to 63

M13_octanol concentration factor 0.706
Carbonate 0.1381 mM
Acidity error 2.26901 mM

Warnings and errors

Errors None
Warnings One or more logP values out of range

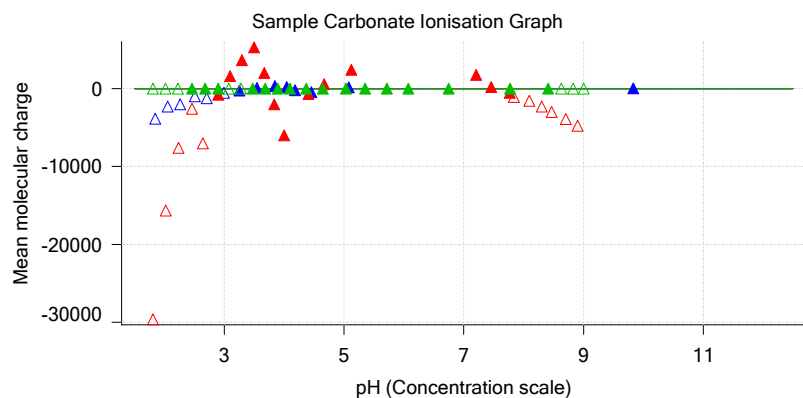
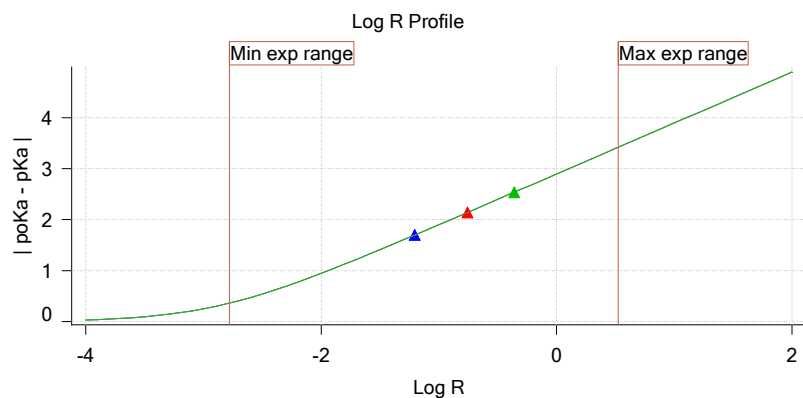
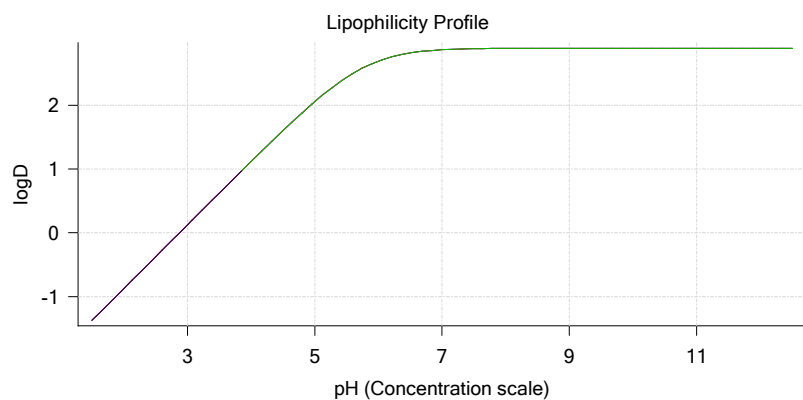
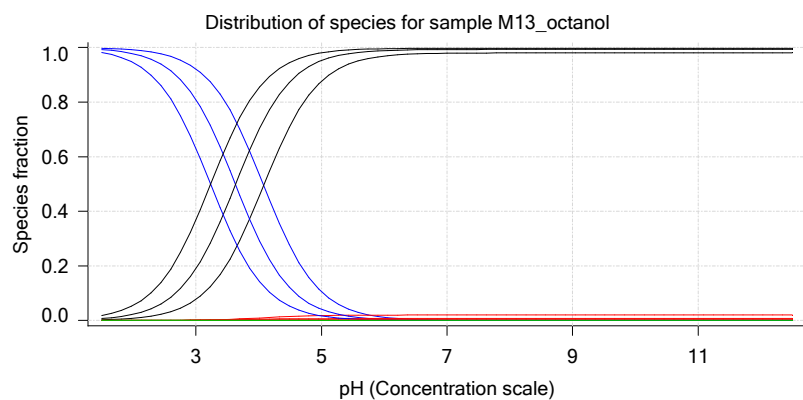
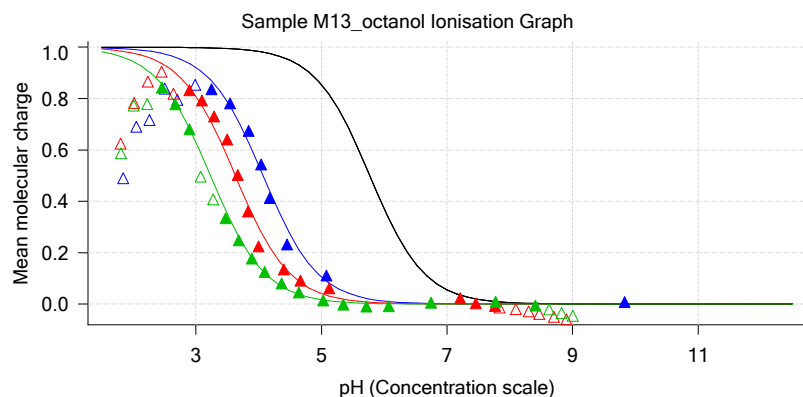
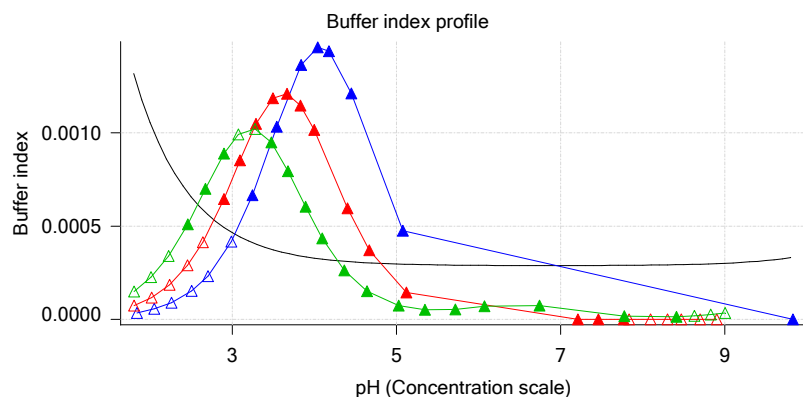
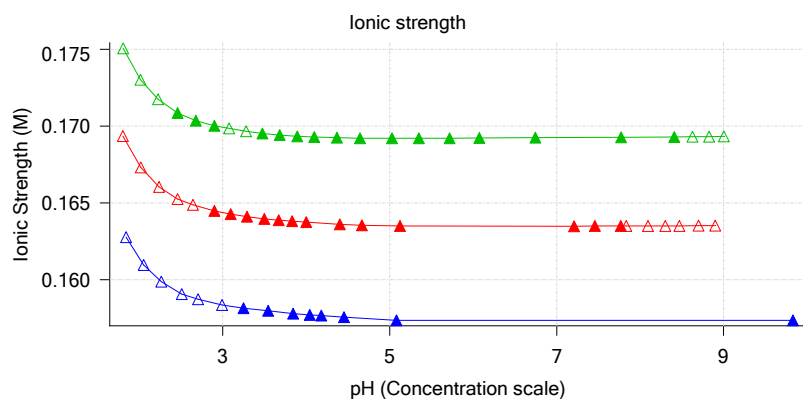
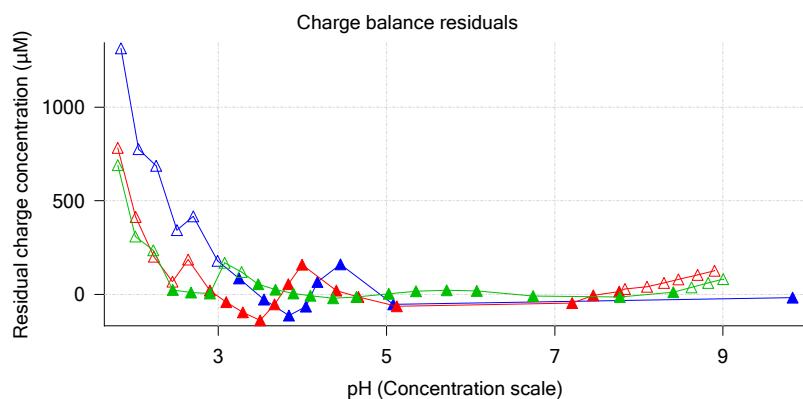
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanol	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.88	98.68 %	0.00 %	0.00 %	1.31 %	Stomach pH
1.200	-1.68	97.93 %	0.00 %	0.00 %	2.07 %	
2.000	-0.88	88.23 %	0.01 %	0.00 %	11.76 %	
3.000	0.12	42.84 %	0.07 %	0.00 %	57.08 %	
4.000	1.12	6.97 %	0.12 %	0.00 %	92.91 %	
5.000	2.06	0.74 %	0.13 %	0.00 %	99.13 %	Blood pH
6.000	2.69	0.07 %	0.13 %	0.00 %	99.80 %	
6.500	2.82	0.02 %	0.13 %	0.00 %	99.85 %	
7.000	2.87	0.01 %	0.13 %	0.00 %	99.87 %	
7.400	2.88	0.00 %	0.13 %	0.00 %	99.87 %	
8.000	2.89	0.00 %	0.13 %	0.00 %	99.87 %	
9.000	2.89	0.00 %	0.13 %	0.00 %	99.87 %	
10.000	2.89	0.00 %	0.13 %	0.00 %	99.87 %	
11.000	2.89	0.00 %	0.13 %	0.00 %	99.87 %	
12.000	2.89	0.00 %	0.13 %	0.00 %	99.87 %	

Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

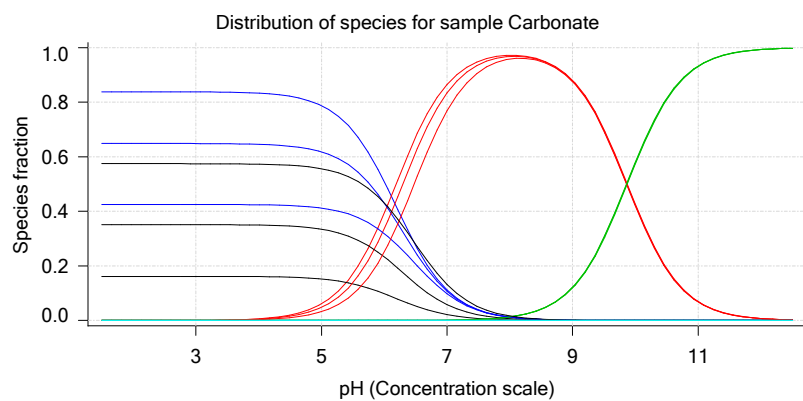
Graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Graphs (continued)



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

pH-metric high logP Titration 1 of 3 18C-16016 Points 2 to 15

Overall results

RMSD 0.073
 Average ionic strength 0.158 M
 Average temperature 24.8°C
 Partition ratio 0.0624 : 1
 Analyte concentration range 2710.7 µM to 2790.7 µM
 Total points considered 8 of 14

Warnings and errors

Errors None
 Warnings One or more logP values out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.167 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 S 0.9932 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 jH 0.7 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 jOH -0.9 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r

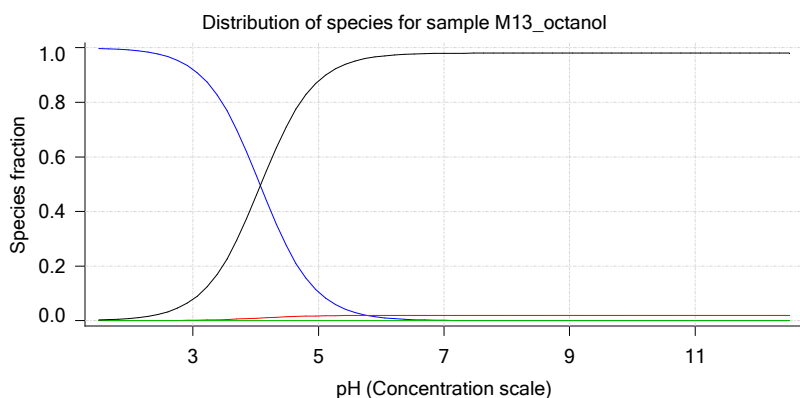
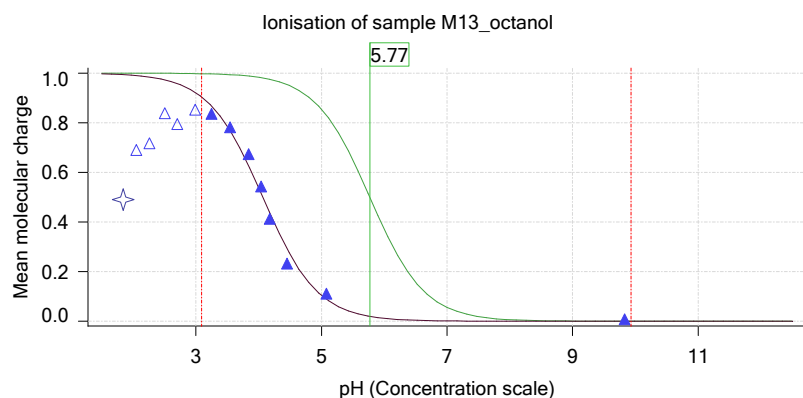
Titrants

0.50 M HCl 0.990198 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 0.50 M KOH 1.009620 3/16/2018 8:34:17 PM C:\Sirius_T3\KOH18C16.t3r

Sample

M13_octanol concentration factor 0.878
 Base pKa 1 5.77
 logP (XH +) -4.56
 logP (neutral X) 2.90

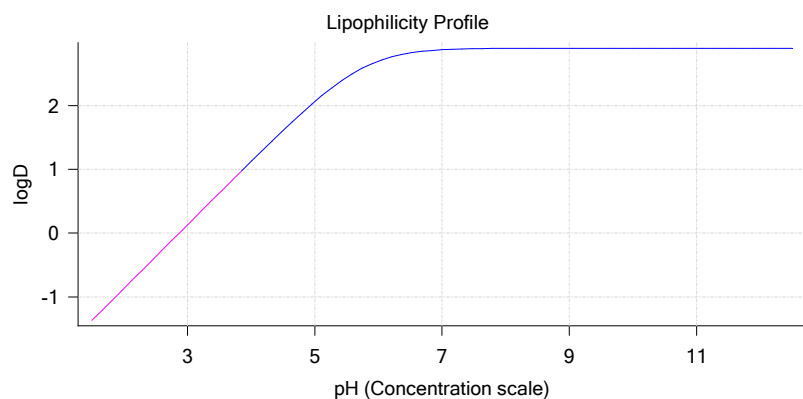
Sample graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Sample graphs (continued)



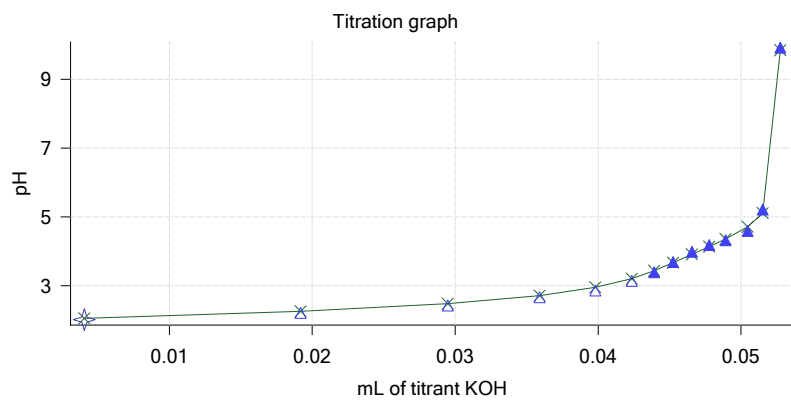
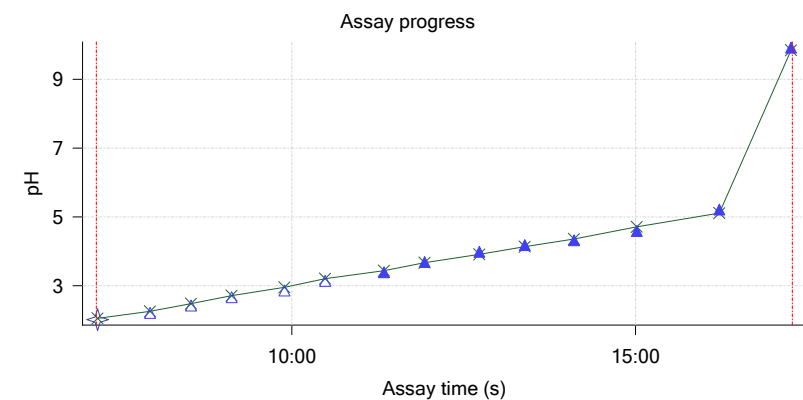
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanolH	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.87	99.91 %	0.00 %	0.00 %	0.08 %	Stomach pH
1.200	-1.67	99.86 %	0.00 %	0.00 %	0.13 %	
2.000	-0.87	99.15 %	0.02 %	0.00 %	0.83 %	
3.000	0.13	92.10 %	0.16 %	0.00 %	7.75 %	
4.000	1.12	53.81 %	0.91 %	0.00 %	45.27 %	
5.000	2.06	10.43 %	1.77 %	0.00 %	87.79 %	Blood pH
6.000	2.70	1.15 %	1.96 %	0.00 %	96.89 %	
6.500	2.83	0.37 %	1.97 %	0.00 %	97.66 %	
7.000	2.87	0.12 %	1.98 %	0.00 %	97.91 %	
7.400	2.89	0.05 %	1.98 %	0.00 %	97.98 %	
8.000	2.90	0.01 %	1.98 %	0.00 %	98.01 %	
9.000	2.90	0.00 %	1.98 %	0.00 %	98.02 %	
10.000	2.90	0.00 %	1.98 %	0.00 %	98.02 %	
11.000	2.90	0.00 %	1.98 %	0.00 %	98.02 %	
12.000	2.90	0.00 %	1.98 %	0.00 %	98.02 %	

Carbonate and acidity

Carbonate 0.000 mM
 Acidity error 2.299 mM

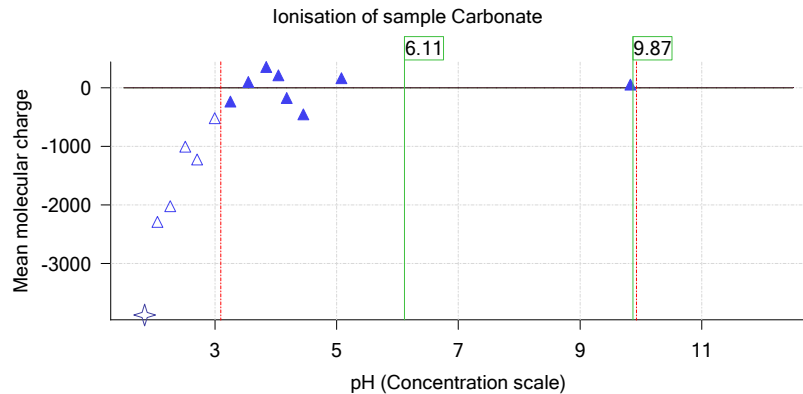
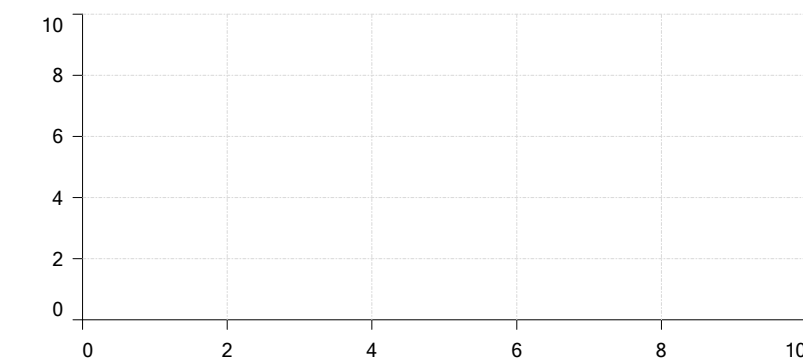
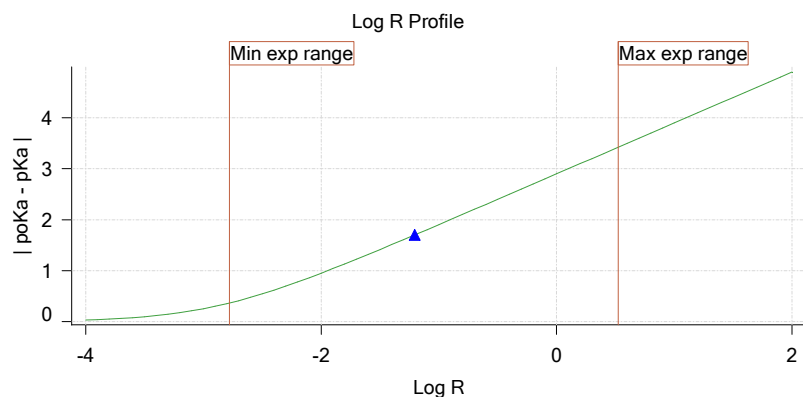
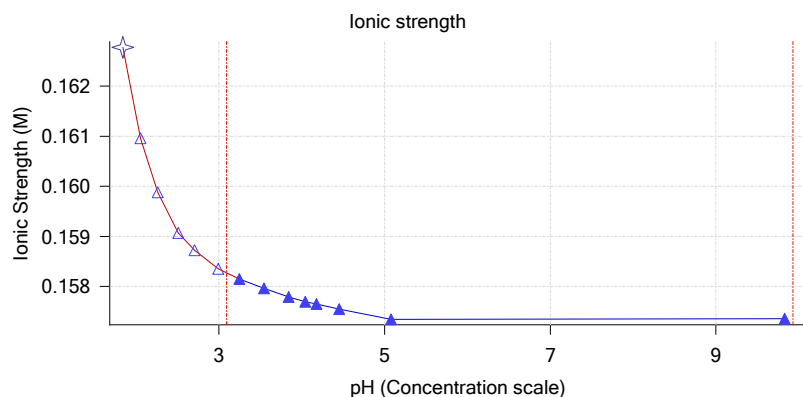
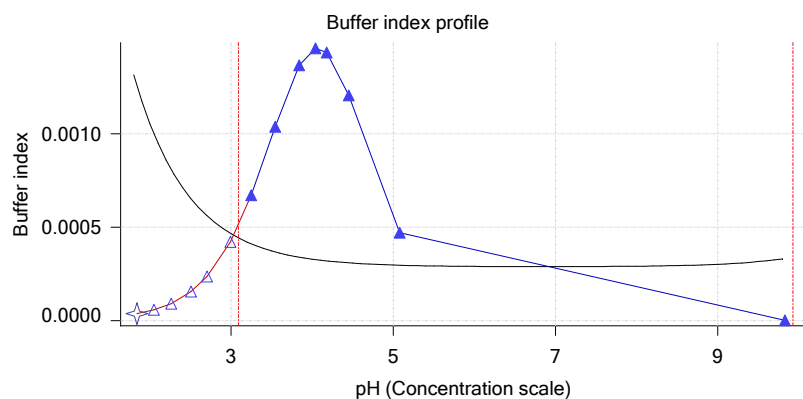
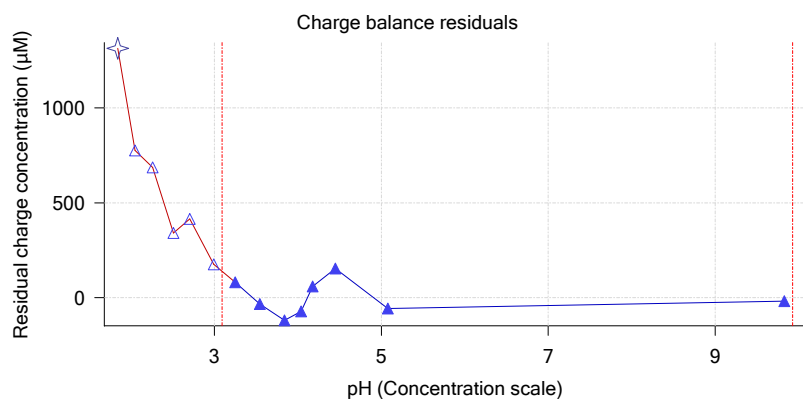
Other graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Other graphs (continued)



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

pH-metric high logP Titration 2 of 3 18C-16016 Points 16 to 39

Overall results

RMSD 6.380
 Average ionic strength 0.164 M
 Average temperature 24.9°C
 Partition ratio 0.1752 : 1
 Analyte concentration range 2287.9 µM to 2354.2 µM
 Total points considered 13 of 24

Warnings and errors

Errors None
 Warnings One or more logP values out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.167 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 S 0.9932 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 jH 0.7 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 jOH -0.9 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r

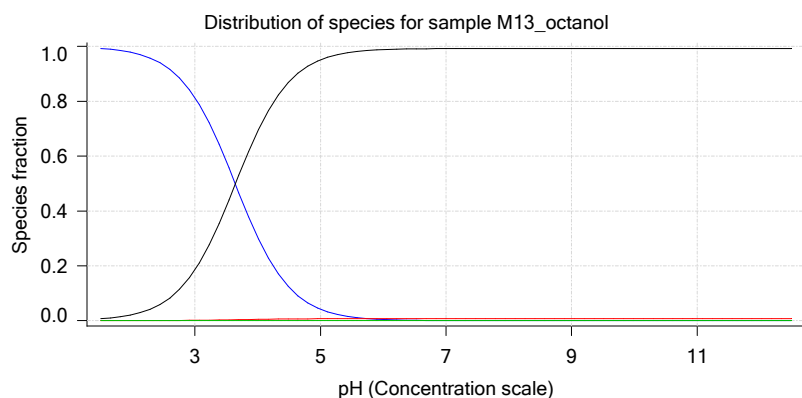
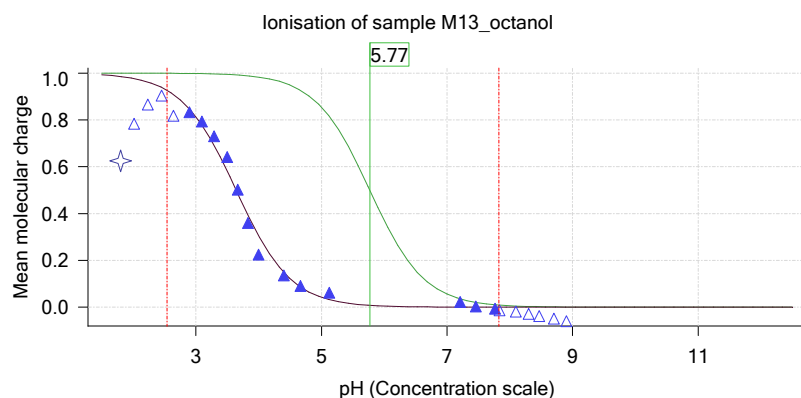
Titrants

0.50 M HCl 0.990198 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 0.50 M KOH 1.009620 3/16/2018 8:34:17 PM C:\Sirius_T3\KOH18C16.t3r

Sample

M13_octanol concentration factor 0.780
 Base pKa 1 5.77
 logP (XH +) -4.56
 logP (neutral X) 2.88

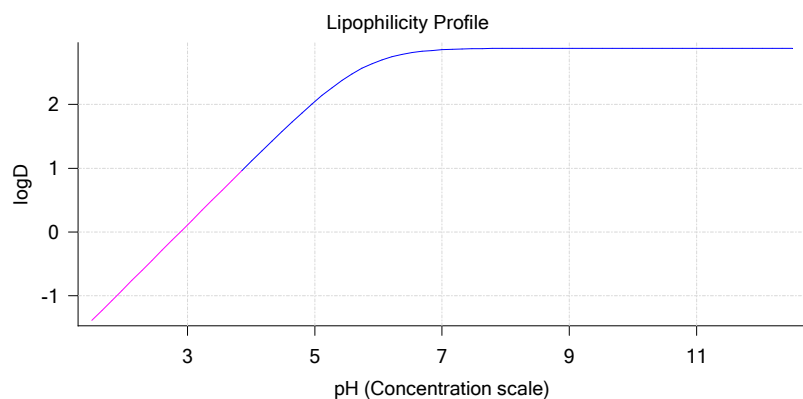
Sample graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Sample graphs (continued)



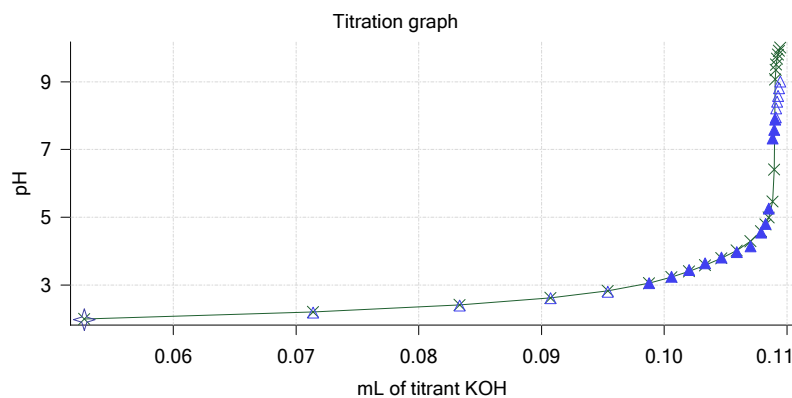
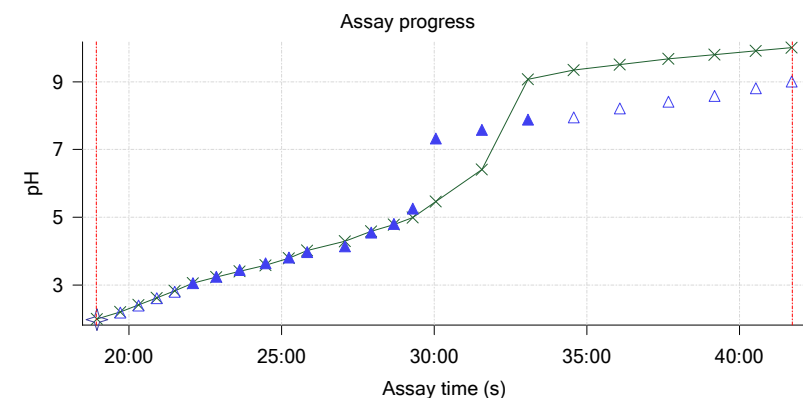
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanolH	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.89	99.77 %	0.00 %	0.00 %	0.23 %	Stomach pH
1.200	-1.69	99.64 %	0.00 %	0.00 %	0.36 %	
2.000	-0.89	97.77 %	0.02 %	0.00 %	2.22 %	
3.000	0.11	81.41 %	0.14 %	0.00 %	18.45 %	
4.000	1.10	30.46 %	0.52 %	0.00 %	69.02 %	
5.000	2.04	4.20 %	0.71 %	0.00 %	95.09 %	Blood pH
6.000	2.68	0.44 %	0.74 %	0.00 %	98.82 %	
6.500	2.81	0.14 %	0.74 %	0.00 %	99.12 %	
7.000	2.86	0.04 %	0.74 %	0.00 %	99.21 %	
7.400	2.87	0.02 %	0.74 %	0.00 %	99.24 %	
8.000	2.88	0.00 %	0.74 %	0.00 %	99.25 %	
9.000	2.88	0.00 %	0.74 %	0.00 %	99.26 %	
10.000	2.88	0.00 %	0.74 %	0.00 %	99.26 %	
11.000	2.88	0.00 %	0.74 %	0.00 %	99.26 %	
12.000	2.88	0.00 %	0.74 %	0.00 %	99.26 %	

Carbonate and acidity

Carbonate 0.000 mM
 Acidity error 2.261 mM

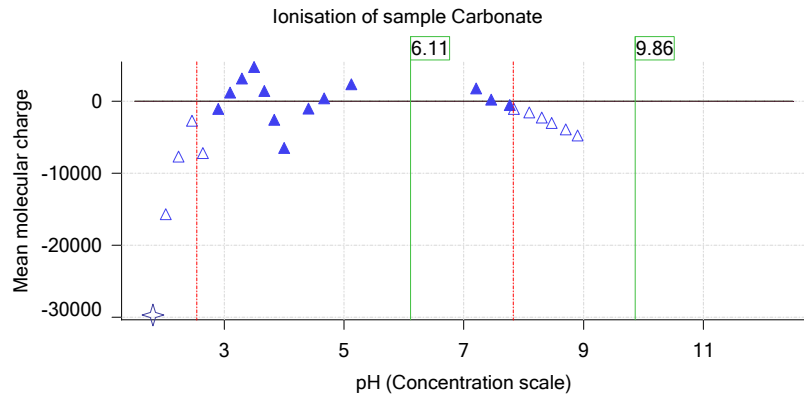
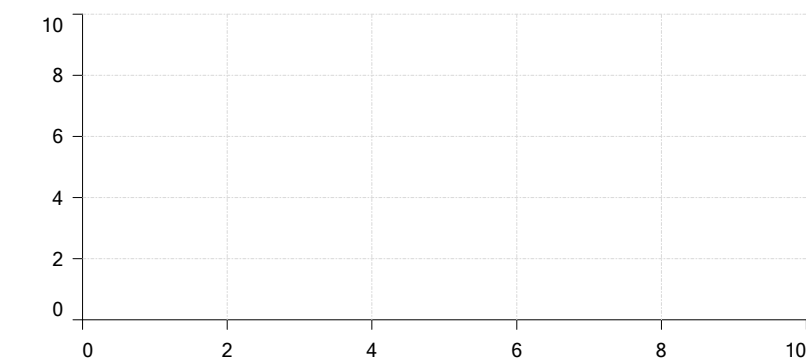
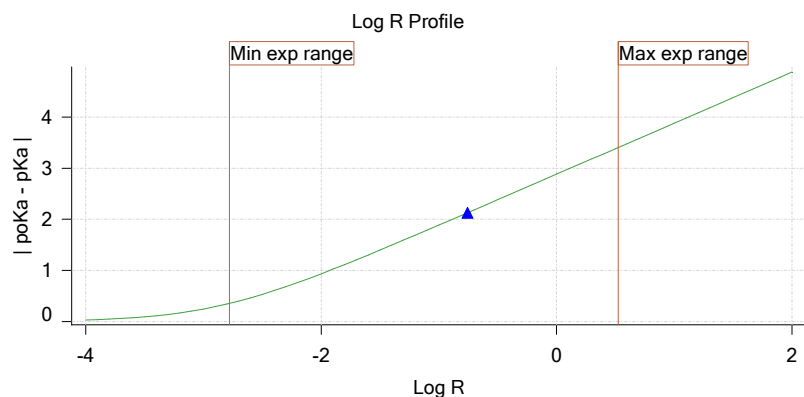
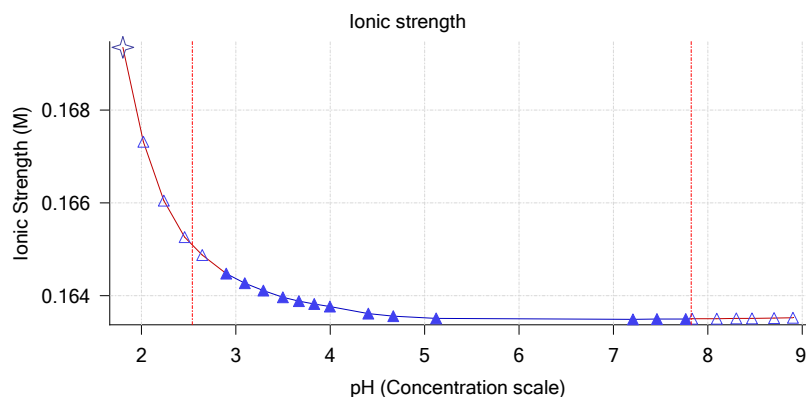
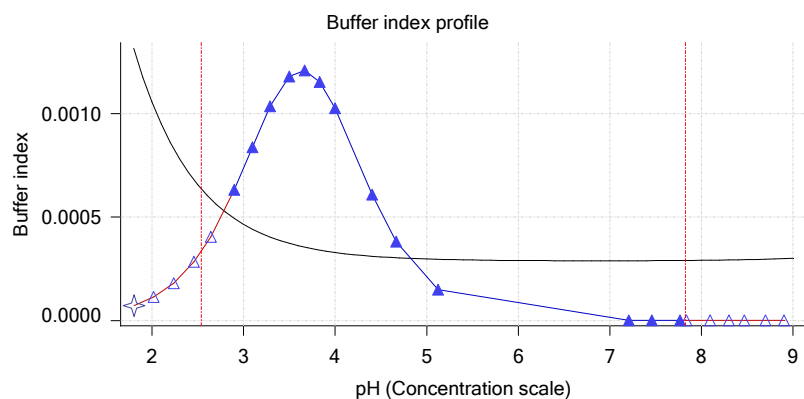
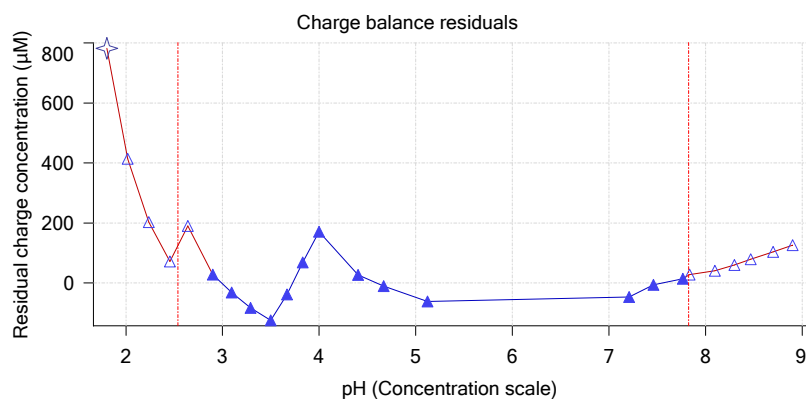
Other graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Other graphs (continued)



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

pH-metric high logP Titration 3 of 3 18C-16016 Points 40 to 63

Overall results

RMSD 0.265
 Average ionic strength 0.169 M
 Average temperature 25.0°C
 Partition ratio 0.4371 : 1
 Analyte concentration range 1749.3 µM to 1790.0 µM
 Total points considered 16 of 24

Warnings and errors

Errors None
 Warnings One or more logP values out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.167 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 S 0.9932 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 jH 0.7 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 jOH -0.9 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r

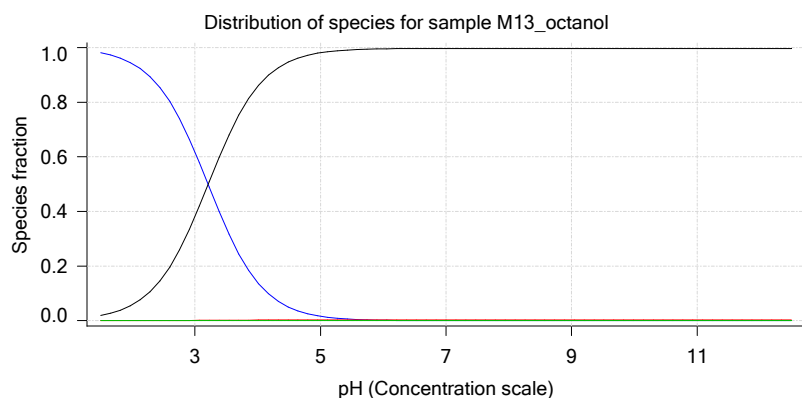
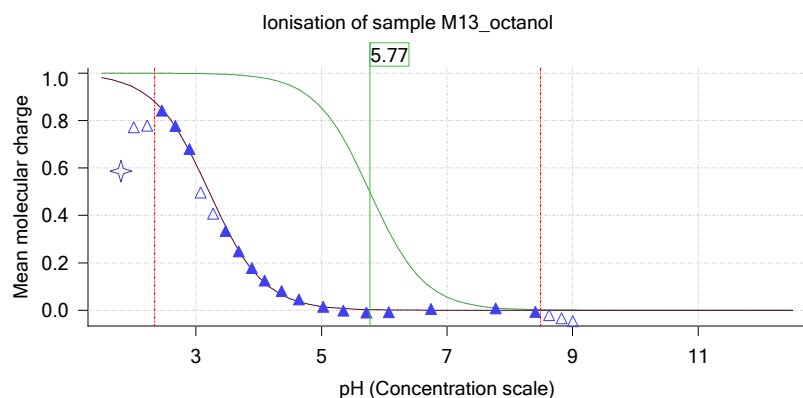
Titrants

0.50 M HCl 0.990198 3/16/2018 8:34:16 PM C:\Sirius_T3\HCl18C16.t3r
 0.50 M KOH 1.009620 3/16/2018 8:34:17 PM C:\Sirius_T3\KOH18C16.t3r

Sample

M13_octanol concentration factor 0.706
 Base pKa 1 5.77
 logP (XH +) -4.56
 logP (neutral X) 2.92

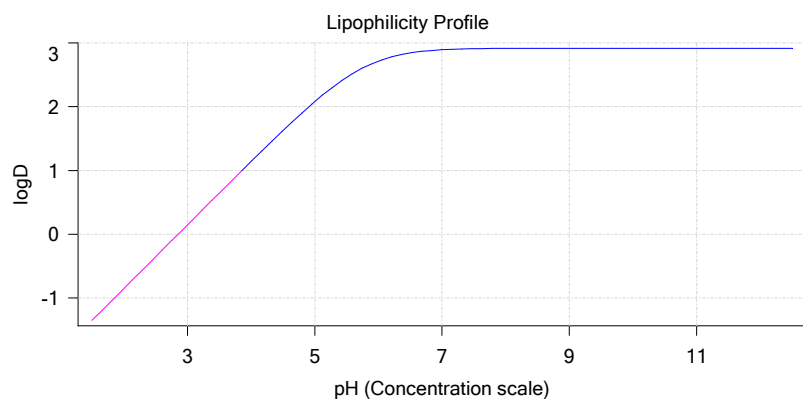
Sample graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**



Sample graphs (continued)



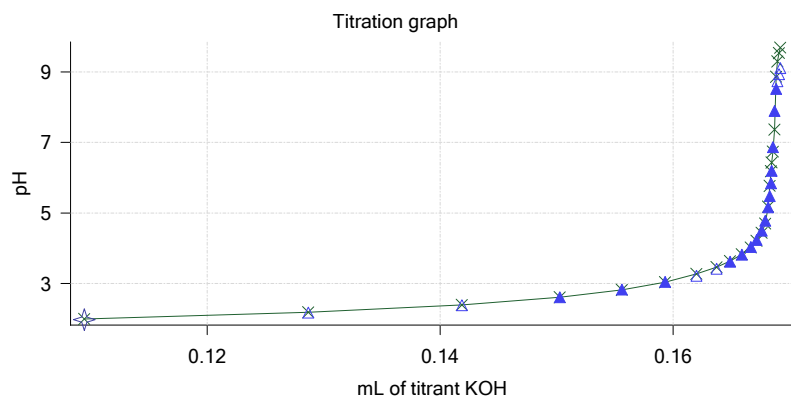
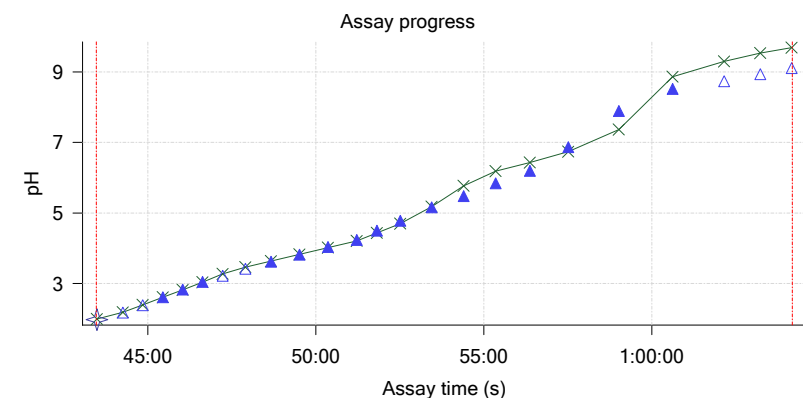
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanolH	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.85	99.39 %	0.00 %	0.00 %	0.61 %	Stomach pH
1.200	-1.65	99.03 %	0.00 %	0.00 %	0.96 %	
2.000	-0.85	94.19 %	0.02 %	0.00 %	5.79 %	
3.000	0.15	61.87 %	0.11 %	0.00 %	38.02 %	
4.000	1.14	13.96 %	0.24 %	0.00 %	85.80 %	
5.000	2.08	1.60 %	0.27 %	0.00 %	98.13 %	Blood pH
6.000	2.72	0.16 %	0.28 %	0.00 %	99.56 %	
6.500	2.84	0.05 %	0.28 %	0.00 %	99.67 %	
7.000	2.89	0.02 %	0.28 %	0.00 %	99.71 %	
7.400	2.91	0.01 %	0.28 %	0.00 %	99.72 %	
8.000	2.92	0.00 %	0.28 %	0.00 %	99.72 %	
9.000	2.92	0.00 %	0.28 %	0.00 %	99.72 %	
10.000	2.92	0.00 %	0.28 %	0.00 %	99.72 %	
11.000	2.92	0.00 %	0.28 %	0.00 %	99.72 %	
12.000	2.92	0.00 %	0.28 %	0.00 %	99.72 %	

Carbonate and acidity

 Carbonate 0.138 mM
 Acidity error 2.269 mM

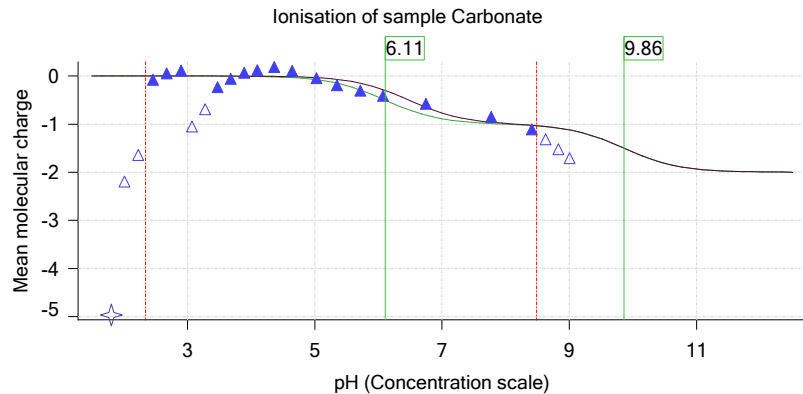
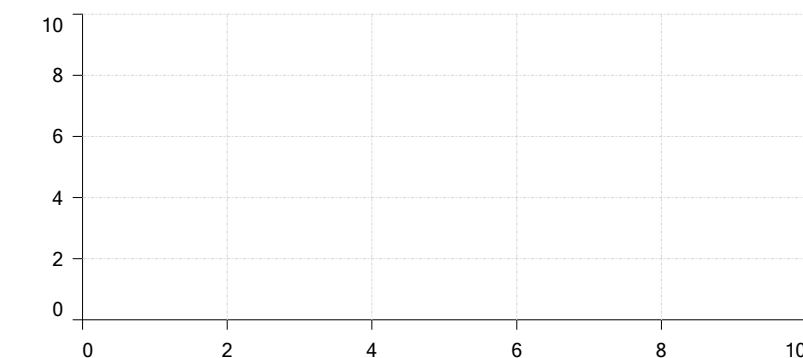
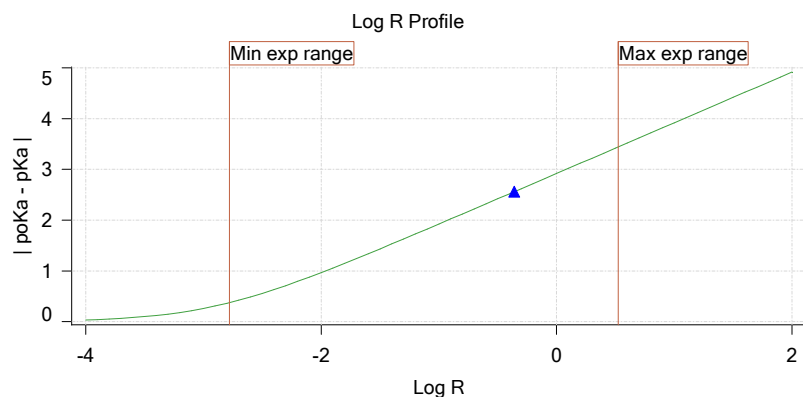
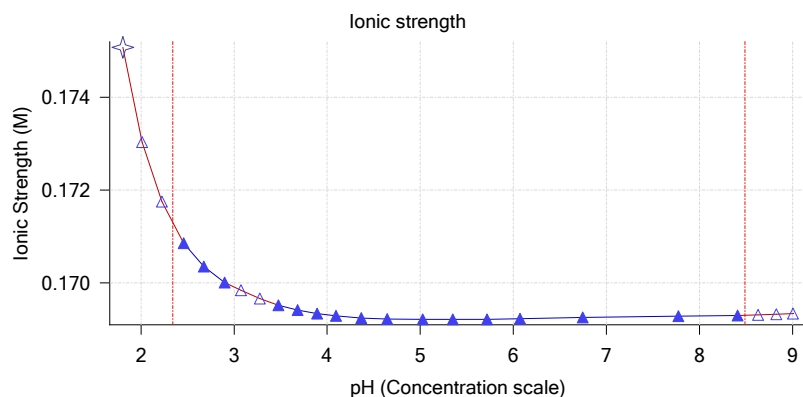
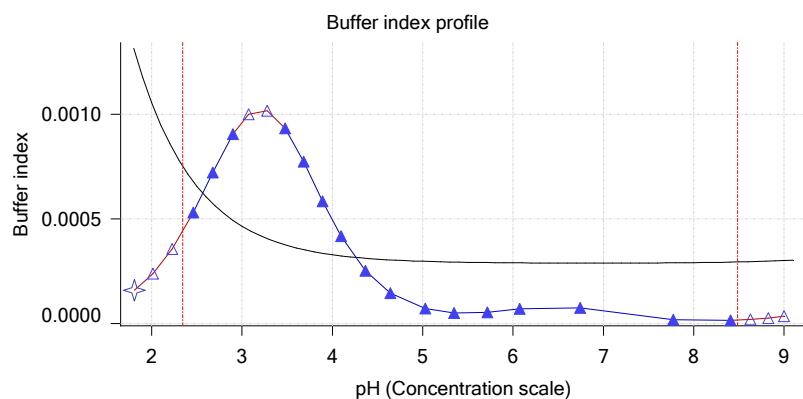
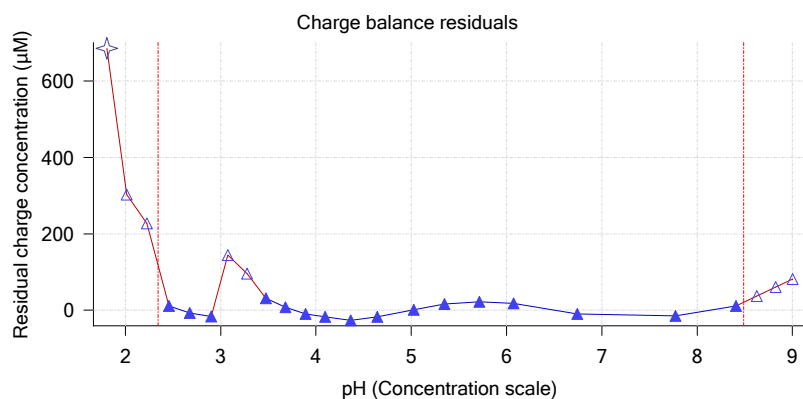
Other graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Other graphs (continued)





Assay model

Sample name: **M13_octanol** Experiment start time: **3/16/2018 8:34:17 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-16016** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M13_octanol	2/27/2018 5:57:49 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001360 g	3/16/2018 5:08:03 PM	User entered value
Formula weight	295.34 g/mol	2/27/2018 5:57:49 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	295.34	2/27/2018 5:57:49 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 5:57:49 PM	User entered value
Sample is a	Base	2/27/2018 5:57:49 PM	User entered value
pKa 1	5.77	2/27/2018 5:57:49 PM	User entered value
logp (XH +)	-4.56	3/2/2018 4:30:48 PM	User entered value
logP (neutral X)	2.99	3/2/2018 4:30:43 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/ time
4:09.8	Manual volume addition				0.10000 mL					
4:10.9	Initial pH = 3.69									
7:10.4	Data point 2	1.50000 mL	0.04605 mL	0.00405 mL	0.10000 mL	2.007	0.00659	0.78015	0.00037	10.0 s
7:56.4	Data point 3	1.50000 mL	0.04605 mL	0.01919 mL	0.10000 mL	2.211	0.00314	0.24211	0.00032	10.0 s
8:32.1	Data point 4	1.50000 mL	0.04605 mL	0.02949 mL	0.10000 mL	2.417	-0.01053	0.38713	0.00084	10.0 s
9:07.7	Data point 5	1.50000 mL	0.04605 mL	0.03591 mL	0.10000 mL	2.660	-0.00938	0.73483	0.00054	10.0 s
9:53.5	Data point 6	1.50000 mL	0.04605 mL	0.03982 mL	0.10000 mL	2.855	-0.00211	0.30085	0.00019	10.0 s
10:29.0	Data point 7	1.50000 mL	0.04605 mL	0.04236 mL	0.10000 mL	3.139	-0.00782	0.88102	0.00041	10.5 s
11:20.4	Data point 8	1.50000 mL	0.04605 mL	0.04393 mL	0.10000 mL	3.394	-0.00736	0.41781	0.00056	10.0 s
11:55.9	Data point 9	1.50000 mL	0.04605 mL	0.04525 mL	0.10000 mL	3.686	-0.01800	0.93937	0.00092	12.0 s
12:43.6	Data point 10	1.50000 mL	0.04605 mL	0.04657 mL	0.10000 mL	3.982	-0.01971	0.97981	0.00098	14.5 s
13:23.6	Data point 11	1.50000 mL	0.04605 mL	0.04779 mL	0.10000 mL	4.181	-0.01960	0.95605	0.00099	17.5 s
14:06.5	Data point 12	1.50000 mL	0.04605 mL	0.04892 mL	0.10000 mL	4.317	-0.01919	0.90540	0.00100	19.0 s
15:01.2	Data point 13	1.50000 mL	0.04605 mL	0.05047 mL	0.10000 mL	4.588	-0.01947	0.95881	0.00098	36.5 s
16:13.4	Data point 14	1.50000 mL	0.04605 mL	0.05153 mL	0.10000 mL	5.212	0.01166	0.44692	0.00086	32.0 s
17:16.0	Data point 15	1.50000 mL	0.04605 mL	0.05275 mL	0.10000 mL	9.929	-0.01846	0.92278	0.00095	43.5 s
18:57.2	Data point 16	1.50000 mL	0.10329 mL	0.05275 mL	0.30000 mL	1.971	-0.00110	0.01132	0.00051	10.0 s
19:43.4	Data point 17	1.50000 mL	0.10329 mL	0.07140 mL	0.30000 mL	2.179	0.00116	0.00555	0.00077	10.0 s
20:19.1	Data point 18	1.50000 mL	0.10329 mL	0.08333 mL	0.30000 mL	2.393	-0.00552	0.08741	0.00092	10.0 s
20:54.7	Data point 19	1.50000 mL	0.10329 mL	0.09073 mL	0.30000 mL	2.610	-0.00664	0.54896	0.00044	10.0 s
21:30.3	Data point 20	1.50000 mL	0.10329 mL	0.09541 mL	0.30000 mL	2.793	-0.01670	0.91771	0.00086	10.5 s



Assay Events

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-16016**
Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
Analyst: **Pion**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
22:06.3	Data point 21	1.50000 mL	0.10329 mL	0.09875 mL	0.30000 mL	3.048	-0.00688	0.24255	0.00069	10.0 s
22:52.1	Data point 22	1.50000 mL	0.10329 mL	0.10059 mL	0.30000 mL	3.242	-0.00986	0.45925	0.00072	10.0 s
23:37.8	Data point 23	1.50000 mL	0.10329 mL	0.10202 mL	0.30000 mL	3.436	-0.00502	0.22328	0.00052	10.0 s
24:28.7	Data point 24	1.50000 mL	0.10329 mL	0.10332 mL	0.30000 mL	3.641	-0.01457	0.55071	0.00097	10.0 s
25:14.5	Data point 25	1.50000 mL	0.10329 mL	0.10466 mL	0.30000 mL	3.811	-0.01728	0.77590	0.00097	10.5 s
25:50.4	Data point 26	1.50000 mL	0.10329 mL	0.10590 mL	0.30000 mL	3.972	-0.02006	0.98341	0.00100	33.5 s
27:04.9	Data point 27	1.50000 mL	0.10329 mL	0.10703 mL	0.30000 mL	4.138	-0.01923	0.92979	0.00098	26.0 s
27:56.3	Data point 28	1.50000 mL	0.10329 mL	0.10788 mL	0.30000 mL	4.540	-0.01305	0.56589	0.00086	14.0 s
28:40.9	Data point 29	1.50000 mL	0.10329 mL	0.10826 mL	0.30000 mL	4.803	-0.00985	0.36149	0.00081	12.0 s
29:18.3	Data point 30	1.50000 mL	0.10329 mL	0.10851 mL	0.30000 mL	5.255	-0.01714	0.86889	0.00091	14.5 s
30:03.2	Data point 31	1.50000 mL	0.10329 mL	0.10882 mL	0.30000 mL	7.326	-0.14623	0.99588	0.00723	Timed out at 59.5 s
31:33.7	Data point 32	1.50000 mL	0.10329 mL	0.10896 mL	0.30000 mL	7.576	-0.08507	0.99600	0.00421	Timed out at 59.5 s
33:04.1	Data point 33	1.50000 mL	0.10329 mL	0.10903 mL	0.30000 mL	7.881	-0.07193	0.99419	0.00357	Timed out at 59.5 s
34:34.5	Data point 34	1.50000 mL	0.10329 mL	0.10908 mL	0.30000 mL	7.949	-0.04523	0.99327	0.00224	Timed out at 59.5 s
36:05.0	Data point 35	1.50000 mL	0.10329 mL	0.10913 mL	0.30000 mL	8.208	-0.03919	0.98798	0.00195	Timed out at 59.5 s
37:40.6	Data point 36	1.50000 mL	0.10329 mL	0.10920 mL	0.30000 mL	8.410	-0.02748	0.97538	0.00137	Timed out at 59.5 s
39:11.0	Data point 37	1.50000 mL	0.10329 mL	0.10927 mL	0.30000 mL	8.578	-0.01916	0.95293	0.00097	45.5 s
40:32.1	Data point 38	1.50000 mL	0.10329 mL	0.10936 mL	0.30000 mL	8.808	-0.01860	0.93287	0.00095	40.0 s
41:42.6	Data point 39	1.50000 mL	0.10329 mL	0.10945 mL	0.30000 mL	9.007	-0.01934	0.95051	0.00098	26.0 s
43:28.9	Data point 40	1.50000 mL	0.16319 mL	0.10945 mL	0.80000 mL	1.973	-0.00097	0.00987	0.00048	10.0 s
44:15.2	Data point 41	1.50000 mL	0.16319 mL	0.12869 mL	0.80000 mL	2.174	-0.01641	0.68236	0.00098	10.0 s
44:50.9	Data point 42	1.50000 mL	0.16319 mL	0.14189 mL	0.80000 mL	2.382	-0.00586	0.20619	0.00064	10.0 s
45:26.6	Data point 43	1.50000 mL	0.16319 mL	0.15028 mL	0.80000 mL	2.612	-0.00646	0.51998	0.00044	10.0 s
46:02.1	Data point 44	1.50000 mL	0.16319 mL	0.15562 mL	0.80000 mL	2.826	-0.01012	0.47373	0.00073	10.0 s
46:37.6	Data point 45	1.50000 mL	0.16319 mL	0.15931 mL	0.80000 mL	3.047	-0.00998	0.83294	0.00054	10.5 s
47:13.6	Data point 46	1.50000 mL	0.16319 mL	0.16202 mL	0.80000 mL	3.221	-0.00942	0.29407	0.00086	10.0 s
47:54.2	Data point 47	1.50000 mL	0.16319 mL	0.16373 mL	0.80000 mL	3.423	-0.00386	0.10317	0.00059	10.0 s
48:39.8	Data point 48	1.50000 mL	0.16319 mL	0.16491 mL	0.80000 mL	3.619	-0.00709	0.28131	0.00066	10.0 s
49:30.7	Data point 49	1.50000 mL	0.16319 mL	0.16592 mL	0.80000 mL	3.823	-0.01281	0.70214	0.00075	10.0 s
50:21.6	Data point 50	1.50000 mL	0.16319 mL	0.16667 mL	0.80000 mL	4.033	-0.00051	0.00324	0.00044	10.5 s
51:12.9	Data point 51	1.50000 mL	0.16319 mL	0.16719 mL	0.80000 mL	4.236	-0.00921	0.79034	0.00051	10.5 s
51:48.8	Data point 52	1.50000 mL	0.16319 mL	0.16761 mL	0.80000 mL	4.504	-0.01403	0.68052	0.00084	11.5 s
52:30.8	Data point 53	1.50000 mL	0.16319 mL	0.16792 mL	0.80000 mL	4.779	-0.01789	0.81440	0.00098	25.5 s
53:26.7	Data point 54	1.50000 mL	0.16319 mL	0.16818 mL	0.80000 mL	5.161	-0.01713	0.81703	0.00093	21.5 s
54:23.9	Data point 55	1.50000 mL	0.16319 mL	0.16832 mL	0.80000 mL	5.480	-0.01521	0.57942	0.00099	21.5 s
55:21.0	Data point 56	1.50000 mL	0.16319 mL	0.16842 mL	0.80000 mL	5.844	-0.01837	0.87683	0.00097	30.5 s
56:22.0	Data point 57	1.50000 mL	0.16319 mL	0.16849 mL	0.80000 mL	6.198	-0.01775	0.86830	0.00094	38.0 s
57:30.5	Data point 58	1.50000 mL	0.16319 mL	0.16858 mL	0.80000 mL	6.865	-0.07156	0.99469	0.00354	Timed out at 59.5 s
59:00.9	Data point 59	1.50000 mL	0.16319 mL	0.16872 mL	0.80000 mL	7.887	-0.09593	0.99713	0.00475	Timed out at 59.5 s
1:00:36.6	Data point 60	1.50000 mL	0.16319 mL	0.16886 mL	0.80000 mL	8.519	-0.01911	0.89364	0.00100	56.5 s
1:02:08.7	Data point 61	1.50000 mL	0.16319 mL	0.16898 mL	0.80000 mL	8.736	-0.01754	0.87325	0.00093	29.0 s
1:03:13.4	Data point 62	1.50000 mL	0.16319 mL	0.16910 mL	0.80000 mL	8.932	-0.01508	0.70146	0.00089	20.5 s
1:04:09.5	Data point 63	1.50000 mL	0.16319 mL	0.16921 mL	0.80000 mL	9.107	-0.01562	0.77923	0.00087	14.5 s
1:04:33.0	Assay volumes	1.50000 mL	0.16319 mL	0.16921 mL	0.80000 mL					

Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.100 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-16016**
Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
Analyst: **Pion**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.500 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.167	3/16/2018 8:34:16 PM	C:\Sirius_T3\HCl18C16.t3r
Four-Plus S	0.9932	3/16/2018 8:34:16 PM	C:\Sirius_T3\HCl18C16.t3r
Four-Plus jH	0.7	3/16/2018 8:34:16 PM	C:\Sirius_T3\HCl18C16.t3r
Four-Plus jOH	-0.9	3/16/2018 8:34:16 PM	C:\Sirius_T3\HCl18C16.t3r
Base concentration factor	1.010	3/16/2018 8:34:17 PM	C:\Sirius_T3\KOH18C16.t3r
Acid concentration factor	0.990	3/16/2018 8:34:16 PM	C:\Sirius_T3\HCl18C16.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	2-6-18	3/5/2018 11:53:26 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	03-16-2018	3/16/2018 11:26:11 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	09-22-17	3/16/2018 11:19:32 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	03-16-2018	3/16/2018 11:40:37 AM
Port B	Cyclohexane		1/16/2018 1:42:16 PM
Port C	MeCN (50%, 0.15 M KCl)	10-30-17	3/16/2018 11:52:45 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	1-31-2018	2/28/2018 10:07:18 AM

Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-16016**
 Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/16/2018 8:34:17 PM**
 Analyst: **Pion**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	1-31-2018	1/31/2018 5:24:59 PM
Titration		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-10.42 mV		3/16/2018 8:34:44 PM
Filling solution	3M KCl	KCL095	3/16/2018 11:15:26 AM
Liquids			
Wash 1	50% IPA:50% Water		3/16/2018 11:15:44 AM
Wash 2	0.5% Triton X-100 in H2O		3/16/2018 11:15:47 AM
Buffer position 1	pH7 Wash		3/16/2018 11:15:49 AM
Buffer position 2	pH 7		3/16/2018 11:15:51 AM
Storage position			3/16/2018 11:16:23 AM
Wash water	4.3e+003 mL	2-27-18	2/27/2018 10:29:26 AM
Waste	5.9e+003 mL		2/27/2018 10:29:30 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	804:59:49		11/23/2010 12:22:28 PM
Calibrated on	2/22/2018 5:36:24 PM		
Integration time	17		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		



Assay Settings

Sample name: **M13_octanol** Experiment start time: **3/16/2018 8:34:17 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-16016** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20180316_exp32_logP_T3-1\18C-16016_M13_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00